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Theoretical Results of One Class of Multiderivative Methods through Order Stars

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Abstract: Order stars are applied to Brown (K, L) methods. They are displayed pictorially for a selection of methods and are used to provide succinct proofs of existing results. Asymptotic results concerning their stability are also presented.

Key Words: Brown (K, L) Methods; Stability; Characteristic Polynomials; Order Stars

1. BROWN METHODS

For the differential equation $y' = f(x, y)$, $y = y(x)$, and fixed integers, K and L , the Brown (K, L) methods^[1] are defined by

$$\sum_{i=0}^K \alpha_i y_{n+i} = \sum_{j=1}^L h^j \beta_j f_{n+K}^{(j-1)}, \quad (1)$$

where the constants α_i and β_j are chosen so as to obtain the highest order possible for the method ($f_{n+K}^{(j)}$ denotes the j -derivative of the function f with respect to x at the point x_{n+K}). Here h denotes the mesh spacing. Jeltsch and Kratz^[2] proved that the coefficients are given by

$$\alpha_i = (-1)^{K-i} \binom{K}{i} (K-i)^{-L}, \quad i = 0, \dots, K-1, \quad \alpha_K = - \sum_{i=0}^{K-1} \alpha_i, \quad (2)$$

$$\beta_j = \frac{(-1)^j}{j!} \sum_{i=0}^{K-1} (-1)^{K-i} \binom{K}{i} (K-i)^{j-L}, \quad j = 1, \dots, L. \quad (3)$$

For $L = 1$, Brown (K, L) methods reduce to the Backward Differentiation Formulae known as BDF methods; these were the first numerical methods to be proposed for stiff differential equations^[3].

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The addition of derivatives in numerical methods gives more scope for better stability characteristics, such as larger regions of absolute stability^[4]. Even though the computation of derivatives is expensive, the combination of the use of higher derivatives and other methods can produce new and improved methods^[5]. For this reason, we study the stability of Brown methods through the theory of order stars; although little used in the literature, this new tool enables the stability of numerical methods to be analysed in a more concise and, arguably, more elegant way.

The Brown (K, L) methods may be represented by their characteristic polynomials

$$\rho(z) = \sum_{i=0}^K \alpha_i z^i \text{ and } \sigma_j(z) = \beta_j z^K, \quad j = 1, 2, \dots, L. \quad (4)$$

A method is zero-stable if the zeros of the polynomial $\rho(z)$ are in the unit disc and the zeros of modulus one are simple. Further, a method is said to be zero-unstable if it is not zero-stable. Here we have been essentially concerned with stability as the mesh spacing h tends to zero. Stability is also of interest in a practical situation when h is fixed, but when we would like the solution to remain bounded or tend to zero as n , the number of steps, increases indefinitely. To study “fixed step” stability the difference equation is often applied to the linear test equation $y' = \lambda y$ resulting in, for linear multistep methods, the characteristic polynomial

$$\pi(w, z) = \rho(z) - z\sigma(z), \quad z = h\lambda. \quad (5)$$

For multiderivative methods the corresponding characteristic polynomial is

$$\pi(w, z) = \rho(z) - \sum_{j=1}^L z^j \sigma_j(w), \quad z = h\lambda. \quad (6)$$

The stability of multistep multiderivative methods depends on the roots $w_i(z)$, $1 \leq i \leq k$ of $\pi(w, z) = 0$. Note that $\pi(w, z) \rightarrow \rho(z)$ as $h \rightarrow 0$ and $w_i(h) \rightarrow w_i$, $1 \leq i \leq k$, where $\{w_i\}$ are the zeros of $\rho(w)$. For a multiderivative method to be consistent, $\rho(1) = 0$ is required. This zero, represented by $w_1(h)$, may be regarded as the principal branch of $\pi(w, z) = 0$ since $w_1(h) \rightarrow w_1$ as $h \rightarrow 0$.

Definition 1.1 *The set $D = \{z \in \overline{\mathbb{C}} / |w_i(z)| \leq 1, 1 \leq i \leq k\}$ is called region of absolute stability of the method, where $\overline{\mathbb{C}} = \mathbb{C} \cup \infty$.*

Definition 1.2 *If the set D consists of the whole of the left hand complex plane, then the method is said to be A-stable.*

More details about stability of multiderivative methods can be found in Ref. [6]. The following results are known about Brown (K, L) methods.

Theorem 1.3 (Jeltsch and Kratz^[2]) *The Brown (K, L) methods have order of consistency $p = K + L - 1$.*

Theorem 1.4 (Iserles and Norsett^[7]) *The Brown (K, L) method of order p is A-stable only if $p \leq 2L$. (Clearly this implies $K \leq L + 1$).*

Theorem 1.5 (Jeltsch and Kratz^[2]) *Let L be fixed. The Brown (K, L) methods become zero-unstable for sufficiently large K .*

Theorem 1.6 (Jeltsch and Kratz^[2]) *Let K be fixed. The Brown (K, L) methods become zero-stable for L sufficiently large.*

The purpose of this note is to introduce order stars for Brown (K, L) methods, compute the order stars for a number of Brown methods and then to re-prove Theorems 1.5 and 1.6 succinctly using order stars.

2. ORDER STARS

There are two types of order stars: order stars of the first kind and of the second kind and they have been shown to be related^[7]. Wanner *et al.*^[8] were the first to describe them and a comprehensive account may be found in Ref. [7]. For our purposes we shall only require order stars of the second kind and will therefore only focus on these.

For the Brown (K, L) methods, let

$$R(z) = \frac{\sum_{j=1}^L \sigma_j(e^z) z^{j-1}}{\rho(e^z)}, \quad F(z) = \frac{1}{z}, \quad (7)$$

and

$$\mu(z) = \frac{\sum_{j=1}^L \sigma_j(e^z) z^{j-1}}{\rho(e^z)} - \frac{1}{z}, \quad z \in \mathbb{C}. \quad (8)$$

Furthermore define

$$A_+ := \{z \mid \operatorname{Re}(\mu(z)) > 0\}, \quad (9)$$

$$A_0 := \{z \mid \operatorname{Re}(\mu(z)) = 0\}, \quad (10)$$

$$A_- := \{z \mid \operatorname{Re}(\mu(z)) < 0\}. \quad (11)$$

An order star $\mu(z)$ of the second kind for a Brown (K, L) method is the partition of the complex plane into the triplet $\{A_+, A_0, A_-\}$.

Let D be the stability region of the numerical method, according Definition 1.1. Then we say that R is A -acceptable and the related method is A -stable if $\{z \in \mathbb{C} \mid \operatorname{Re}(z) < 0\} \subset D$.

Definition 2.1 The index $\iota(z)$ of a point $z \in A_0$ is defined as the number of sectors of A_- adjoining z .

Let $z \in A_0$ and $p = \iota(z) > 0$. If μ is analytic at z and the point is approached by precisely p sectors of A_- and p sectors of A_+ , each of asymptotic angle $\frac{\pi}{p}$, then we say that z is regular.

The next result relates the order of the method to the number of sectors forming the regions A_+ and A_- .

Lemma 2.2 If the Brown (K, L) method has order p , then the origin is adjoined by $p - 1$ sectors of A_+ and separated by $p - 1$ sectors of A_- . All these sectors approach the origin with asymptotic angle $\frac{\pi}{p-1}$.

The proof can be found in Ref. [9].

The next result establishes the zero-stability of a (K, L) method through order stars.

Lemma 2.3 Brown methods are zero-stable if, and only if, all the poles of $\mu(z)$ reside in the closed left half-plane and the poles along the imaginary axis are simple.

It is important to remember that, for the proofs of the above results, the use of the transformation $z \rightarrow \ln z$ is required. This maps, of course, the unit disk onto the left half-plane and the unit circle onto the imaginary axis.

The A -stability of a method or, equivalently, the A -acceptability of the approximation μ is given in the following result:

Lemma 2.4 *The approximation μ is A -acceptable if, and only if $A_- \cap \{i\mathbb{R}\} = \emptyset$.*

The proof can be found in Ref. [7].

The function $\mu(z)$ involves e^z , which is periodic in the complex plane. Hence, both zeros and poles are replicated by multiples of $2\pi i$, and this creates obvious difficulties for zero and pole counting arguments. It is therefore, necessary to restrict our attention to the region

$$J = \{z \in \mathbb{C} : |\operatorname{Im}(z)| \leq \pi\}. \quad (12)$$

Let us define the sets

$$J^+ = \{z \in J : \operatorname{Re}(z) > 0\} \text{ and } J^- = \{z \in J : \operatorname{Re}(z) < 0\}. \quad (13)$$

Finally, a closed curve in A_0 will be called a loop.

Lemma 2.5 *There exists $\epsilon \in \mathbb{R}$ such that the set $\{z | \operatorname{Re}(z) \geq \epsilon\} \cap J$ is contained in one of the sets A_+ or A_- : if $\beta_L > 0$ then it belongs to A_+ , otherwise it lies in A_- .*

The proof can be found in Ref. [10].

The next result defines the relative position between the zeros and poles of $\mu(z)$.

Lemma 2.6 *Let δ be a loop such that $\delta \cap \partial J = \emptyset$ and $\delta \cap J \neq \emptyset$. Then, there is on δ exactly one pole of μ between any two roots of $\mu(z) = 0$. Moreover, if $z_0 \in \operatorname{int}(J)$ is a pole of μ of multiplicity m then it is approached by m sectors of A_+ and m sectors of A_- each with asymptotic angle of $\frac{\pi}{m}$.*

Lemma 2.7 *Let G be either a bounded A_+ -region or A_- -region such that $\{\mathbb{R} + i\pi\} \cap \operatorname{cl}(G) \neq \emptyset$ and*

$$x_- = \min\{x \in \mathbb{R} : x + i\pi \in \operatorname{cl}(G)\} > -\infty \quad (14)$$

$$x_+ = \max\{x \in \mathbb{R} : x + i\pi \in \operatorname{cl}(G)\} < \infty. \quad (15)$$

Let $z_0 \in \partial G \cap \operatorname{int}(J)$ be a zero of $\mu(z)$. Then

1. if G is a A_- -region then either $x_- + i\pi$ is a pole of μ or there is a pole of μ along the positively oriented portion of ∂G from $x_- + i\pi$ to z_0 ;
2. if G is a A_+ -region then either $x_+ + i\pi$ is a pole of μ or there is a pole of μ along the positively oriented portion of ∂G from z_0 to $x_+ + i\pi$.

Similar results are valid if $\mathbb{R} + i\pi$ is replaced by $\mathbb{R} - i\pi$.

Lemma 2.8 *Let z_0 be a pole of $\mu(z)$ with multiplicity m . Then $\iota(z_0) = m$ and z_0 is regular.*

Again, the proof of this result may be found in Ref. [7].

3. ORDER STARS FOR THE BROWN (K, L) METHODS

For the BDF methods, we have

$$\mu(z) = \frac{\sigma(e^z)}{\rho(e^z)} - \frac{1}{z} \text{ (equivalent to (8) with } L = 1). \quad (16)$$

For $K = 2$, this results in

$$\mu(z) = \frac{\left(\frac{2}{3}z - 1\right)e^{2z} + \frac{4}{3}e^z - \frac{1}{3}}{z\left(e^{2z} - \frac{4}{3}e^z + \frac{1}{3}\right)}, \quad (17)$$

and for $K = 4$,

$$\mu(z) = \frac{\left(\frac{12}{25}z - 1\right)e^{4z} + \frac{48}{25}e^{3z} - \frac{36}{25}e^{2z} + \frac{16}{25}e^z - \frac{3}{25}}{z\left(e^{4z} - \frac{48}{25}e^{3z} + \frac{36}{25}e^{2z} - \frac{16}{25}e^z + \frac{3}{25}\right)}. \quad (18)$$

Figures 1 and 2 display the order stars for the BDF methods with $K = 2, 3, 4, 6, 7$ and 9 , respectively, in the interval $[-\pi, \pi]$. The dark region represents A_+ and the complementary area represents A_- . In each of these pictures the points in A_0 are the poles of $\mu(z)$ and the point at the origin represents the principal root of $\rho(z) = 0$, that is $z_0 = 1$.

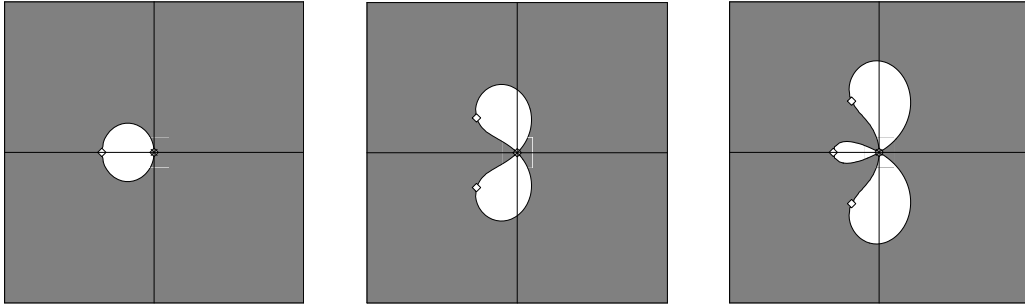


Figure 1: Order star of Brown (2,1), (3,1) and (4,1) methods, respectively

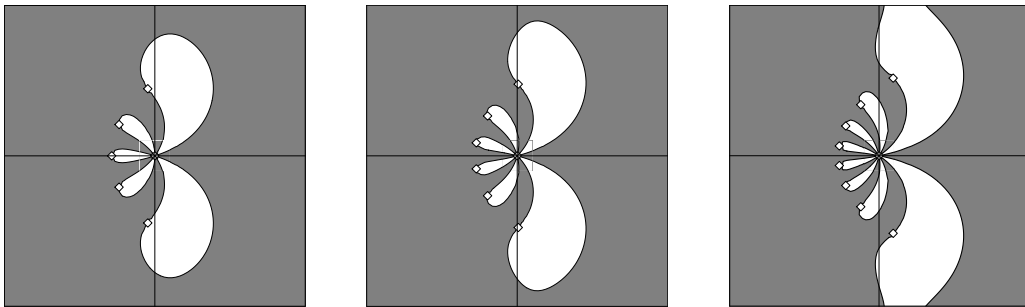


Figure 2: Order star of Brown (6,1), (7,1) and (9,1) methods, respectively

Observe that the order stars of each method has $p - 1 = K - 1$ sectors, where $p = K$ is the order of the method. For $K = 2$, $A_- \cap \{i\mathbb{R}\} = \emptyset$ and for $K \geq 3$, $A_- \cap \{i\mathbb{R}\} \neq \emptyset$. Then, the BDF methods are A -stable only

if $K \leq 2$. For the point $z_0 = 0$ we have $\iota(0) = K - 1$, because $p = K - 1$ and $K - 1$ sectors of A_- approach $z_0 = 0$. So, from Lemma 2.8 it follows that $z_0 = 0$ is regular.

We know that the BDF methods are zero-stable only for $K \leq 6$ (see Hairer and Wanner^[11]). This fact can be observed in Figures 1 and 2 by noting that the poles of $\mu(z)$, for $K = 1, 2, 3, 4, 5$ and 6, lie in the left half-plane. For $K = 7$ and $K = 9$, for example, the methods are zero-unstable.

In the general case, the order stars for the Brown (K, L) methods will have $K + L - 2$ sectors of A_- and $K + L - 2$ sectors of A_+ approaching the origin each with asymptotic angle of $\frac{\pi}{K + L - 2}$, as predicted by Lemma 2.2, because these methods have order $p = K + L - 1$.

From Ref. [12] we know that

$$\begin{aligned} \mu\left(\frac{1}{\xi}\right) &= \frac{\sigma(e^{1/\xi})}{\rho(e^{1/\xi})} - \xi = \frac{\sigma(e^{1/\xi}) - \xi\rho(e^{1/\xi})}{\rho(e^{1/\xi})} \\ &= \frac{e^{K/\xi} \left(\beta_1 + \beta_2 \left(\frac{1}{\xi}\right) + \dots + \beta_L \left(\frac{1}{\xi}\right)^{L-1} \right) - \xi \left(\alpha_0 + \alpha_1 e^{1/\xi} + \dots + \alpha_K e^{K/\xi} \right)}{\alpha_0 + \alpha_1 e^{1/\xi} + \dots + \alpha_K e^{K/\xi}} \\ &= \frac{\beta_1 + \beta_2 \left(\frac{1}{\xi}\right) + \dots + \beta_L \left(\frac{1}{\xi}\right)^{L-1} - \xi \left(\frac{\alpha_0}{e^{K/\xi}} + \dots + \alpha_K \right)}{\frac{\alpha_0}{e^{K/\xi}} + \dots + \alpha_K}. \end{aligned} \quad (19)$$

Then

$$\lim_{\xi \rightarrow 0} \xi^{L-1} \mu\left(\frac{1}{\xi}\right) = \frac{\beta_L}{\alpha_K}, \quad (20)$$

implying that 0 is a pole of order $L - 1$ of $\mu\left(\frac{1}{\xi}\right)$ and $z_0 = \infty$ is a pole of order $L - 1$ of $\mu(z)$.

So, from Lemma 2.8, $\iota(\infty) = L - 1$. Moreover,

$$\iota(0) = K + L - 2 = (K - 1) + (L - 1). \quad (21)$$

Then, $(K - 1) + (L - 1)$ sectors of A_- approach the origin, where $L - 1$ sectors are obtained from $\iota(\infty) = L - 1$ (by Lemma 2.5, these sectors reside in the right half-plane and are unbounded) and $K - 1$ sectors reside in the left half-plane, and contain the poles of the approximation $\mu(z)$ (by the Lemmas 2.6 and 2.7).

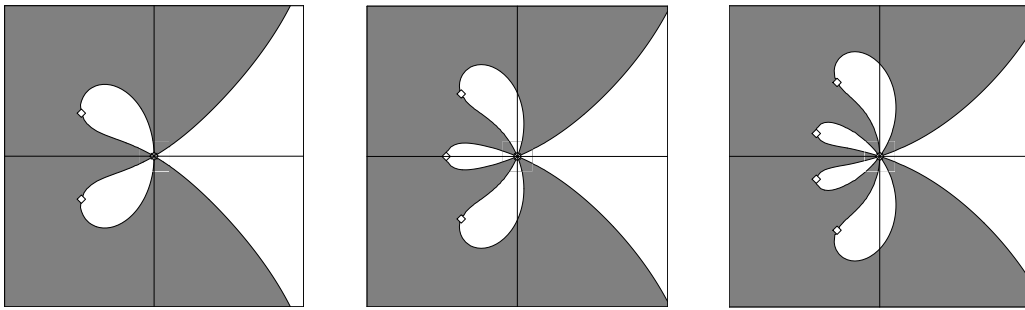


Figure 3: Order star of Brown (3,2), (4,2) and (5,2) methods, respectively

For example, in the case that $L = 2$, $p = K + 1$ and each order star has $p - 1 = K$ sectors we obtain the following. As $\iota(\infty) = 1$, there is one unbounded sector on the right half-plane. For $K = 3$, $A_- \cap \{i\mathbb{R}\} = \emptyset$ and for $K \geq 4$, $A_- \cap \{i\mathbb{R}\} \neq \emptyset$. Then, the $(K, 2)$ methods are A -stable only if $K \leq 3$. The point $z_0 = 0$ is an

interpolation point of degree $p = K$ because K sectors of A_- approach $z_0 = 0$. Moreover, $\iota(0) = K - 1$. So, from Lemma 2.8 it follows that $z_0 = 0$ is regular. From Figures 3 and 4 it may be observed that the poles of $\mu(z)$, for $K = 3, 4, 5, 7$ and 10 , lie in the left half-plane. Then, these methods are zero-stable. For $K = 11$, for example, the method is zero-unstable.

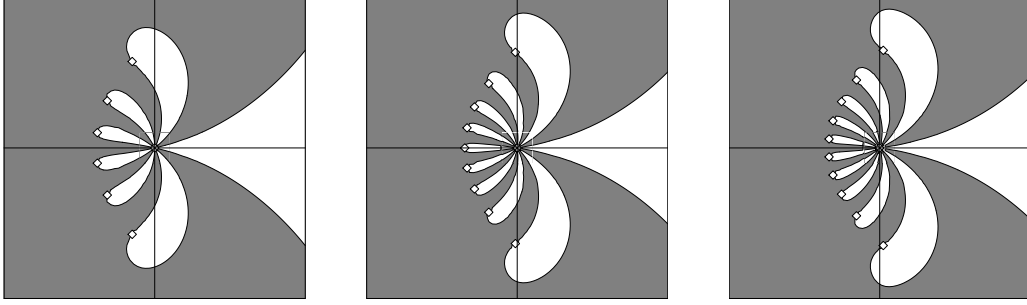


Figure 4: Order star of Brown (7,2), (10,2) and (11,2) methods, respectively

The Figure 5 show the order stars for other values of K and L .

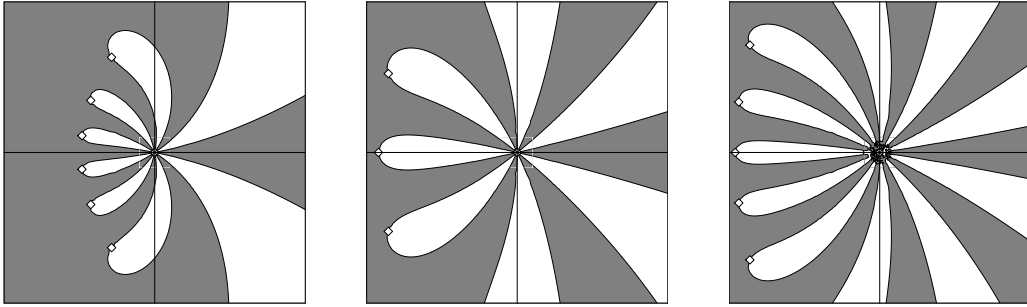


Figure 5: Order star of Brown (7,3), (4,5) and (6,7) methods, respectively

4. TWO ASYMPTOTIC RESULTS

Two asymptotic results concerning zero-stability will be given. Although these were previously discussed by Meneguetto^[4], order stars permit a much more concise proof.

Theorem 4.1 *Let L be fixed. Brown (K, L) methods become zero-unstable for K sufficiently large.*

Proof. Let

$$\mu(z) = \frac{\sum_{j=1}^L \sigma_j(e^z) z^{j-1}}{\rho(e^z)} - \frac{1}{z}, \quad (22)$$

be the generating function of the order stars for the Brown (K, L) methods. Observe that $\iota(\infty) = L - 1$. Then, for the (K, L) method,

$$\iota(0) = (K - 1) + (L - 1) \text{ and } \iota(\infty) = L - 1,$$

and for the $(K + 1, L)$ method,

$$\iota(0) = K + (L - 1) \text{ and } \iota(\infty) = L - 1.$$

This means that, as K increases, the number of loops (which support the zeros of $\rho(z)$) increases with K and $\iota(\infty)$ remains constant. If the (K, L) method are to be zero-stable then, by Lemma 2.3, the loops of the order stars lie in the left half-plane. As the plane is divided by $K + L - 2$ sectors of A_- and $K + L - 2$ sectors of A_+ (by Lemma 2.2), for a sufficiently large K , the loops cross the imaginary axis and then at least one pole of $\mu(z)$ lies in the right half-plane. This characterizes a zero-unstable method.

If the loops in the right half-plane intersect with the left half-plane, when K increases, the loops cross the region $|\operatorname{Im}(z)| \leq \pi$; but the poles of $\mu(z)$ lie in this region (by the Lemmas 2.6 and 2.7) and, consequently, at least one pole lies in the right half-plane. \square

Theorem 4.2 *Let K be fixed. The Brown (K, L) methods become zero-stable for L sufficiently large.*

Proof. Let K be fixed and L sufficiently large. As K is fixed then the number of sectors containing poles remains constant, because each one contains one distinct zero of $\rho(z)$. On the other hand for the (K, L) method,

$$\iota(0) = (K - 1) + (L - 1) \text{ and } \iota(\infty) = L - 1,$$

and for the $(K, L + 1)$ method,

$$\iota(0) = (K - 1) + L \text{ and } \iota(\infty) = L.$$

Hence $\iota(\infty)$ increases with L . As the plane is divided by $K + L - 2$ sectors of A_- and $K + L - 2$ sectors of A_+ (by Lemma 2.2), then for sufficiently large L , the number of sectors from the positive x axis towards the y axis increases (because these sectors reside in the right half-plane). Then, by increasing the number of sectors related to the $\iota(\infty)$ sufficiently, the poles will lie in the left half-plane. This characterizes a zero-stable method.

If the loops in the left half-plane intersect with the right half-plane, when L increases, the loops cross the region $|\operatorname{Im}(z)| \leq \pi$; but the poles of $\mu(z)$ lie in this region and, consequently, for L sufficiently large, the poles will lie in the left half-plane. \square

5. CONCLUSION

This article has introduced order stars as applied to the Brown (K, L) methods. The order stars of a number of Brown (K, L) methods have been computed and displayed pictorially. They then have been used to establish, in a succinct manner, two asymptotic results originally due to Ref. [2].

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